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Morphology of cerium oxide surfaces in an oxidzing enviroment:a first-principles investigation MARCO FRONZI, ALOYSIUS SOON, CATHERINE STAMPFL, School of Physics, University of Sydney, Australia, BERNARD DELLEY, Paul-Sherrer Institute, ENRICO TRAVERSA, University of Tor Vergata, Rome — A good understanding of the stability and chemistry of CeO_2 surfaces is crucial for a better designing of solid oxide fuel cells. As the first step, we use DFT [1] to study the structural and electronic ground state properties of bulk CeO_2. various surface termination of the low-index surface of CeO_2 are then investigated, namely the stoichiometric, metal- and oxygen- rich terminations, and defected surfaces. Using the concept of "*ab initio* atomistic thermodynamics" [2], we calculate the surface free energy phase diagram. This allows us to identify and predict stable, and potentally catalytically important, structures. There is an evidence to suggest an interesting morphological change in the surface structures with varying oxygen concentration. Reaction pathways for methane oxidation on low energy cerium oxide surfaces are being investigated and will be reported.
[1] Formulated in the DMol^3 code; B. Delley, J. Chem. Phys. 92, 508 (1990);ibid. 113, 7756 (2000).
[2] K. Reuter, C. Stampfl and M. Scheffler, in Handbook of Materials Modeling, Volume 1, Fundamental Models and Methods, Sidney Yip (Ed)(2005).

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